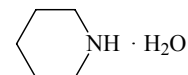


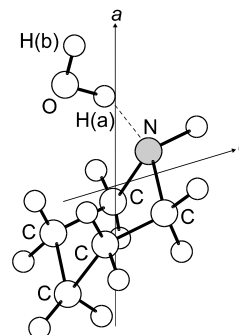
679
MW $\text{C}_5\text{H}_{13}\text{NO}$ **Piperidine – water (1/1)**
(weakly bound complex) C_s
(effective symmetry class)
(large-amplitude motion)

r_0	$\text{\AA}^{\text{a})}$
N...O	2.916(5)

θ_0	$\text{deg}^{\text{a})}$
C–N...H(a)	122.15(50)



The observed spectrum agrees with two possible structures. Only one of them is supported by the dipole moment estimated from line intensities and is consistent with calculations on the MP2/6-31G** level. In this structure the N...H–O hydrogen bond and the water molecule are located in the symmetry plane of piperidine. The free water proton is directed into the same direction as the imino proton.



^{a)} Uncertainties were not estimated in the original paper.

Spoerel, U., Stahl, W.: Chem. Phys. **239** (1998) 97.